THE ROLE OF C^*-ALGEBRAS IN INFINITE DIMENSIONAL NUMERICAL LINEAR ALGEBRA

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Abstract. This paper deals with mathematical issues relating to the computation of spectra of self adjoint operators on Hilbert spaces. We describe a general method for approximating the spectrum of an operator A using the eigenvalues of large finite dimensional truncations of A. The results of several papers are summarized which imply that the method is effective in most cases of interest. Special attention is paid to the Schrödinger operators of one-dimensional quantum systems.

We believe that these results serve to make a broader point, namely that numerical problems involving infinite dimensional operators require a reformulation in terms of C^*-algebras. Indeed, it is only when the given operator A is viewed as an element of an appropriate C^*-algebra $\mathcal{A}$ that one can see the precise nature of the limit of the finite dimensional eigenvalue distributions: the limit is associated with a tracial state on $\mathcal{A}$. For example, in the case where A is the discretized Schrödinger operator associated with a one-dimensional quantum system, $\mathcal{A}$ is a simple C^*-algebra having a unique tracial state. In these cases there is a precise asymptotic result.

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1. Introduction. We discuss methods for computing the spectrum $\sigma(A)$, and especially the essential spectrum $\sigma_e(A)$, of bounded self-adjoint operators A on separable Hilbert spaces.

We mean to take the term 'compute' seriously. Most operators that arise in practice are not presented in a representation in which they are diagonalized, and it is often very hard to locate even a single point in the spectrum of the operator [6], [7], [8], [12], [13], [15]. Some typical examples will be discussed in section 3. Thus, one often has to settle for numerical approximations to $\sigma(A)$ or $\sigma_e(A)$, and this raises the question of how to implement the methods of finite dimensional numerical linear algebra to compute the spectra of infinite dimensional operators. Unfortunately, there is a dearth of literature on this basic problem and, so far as we have been able to tell, there are no *proven* techniques.

In this paper we establish an effective method for approaching such problems; we discuss issues associated with operator theory and operator algebras, but not issues belonging properly to numerical analysis. Thus, we address the question of whether or not certain finite dimensional approximations converge to the correct limit, but we do not address questions relating to how fast they converge nor how this method might be implemented algorithmically. Nevertheless, it may be appropriate to point out that these methods have been effectively implemented in a Macintosh program [2] which is available from the author.

The following section contains a general method for computing the essential spectrum of a self adjoint operator. The method depends on choosing an orthonormal basis and approximating the operator with $n \times n$ matrices obtained as sections of the infinite matrix of the operator with respect to this basis. Not every orthonormal basis is appropriate, and we develop criteria which show how the basis must be chosen. This involves an abstraction of the classical notion of band-limited matrix.

Our method is effective for computing the essential spectrum. When there is a difference between the spectrum and essential spectrum, our results give no information about points in the difference $\sigma(A) \setminus \sigma_e(A)$. However, since $\sigma(A) \setminus \sigma_e(A)$ consists merely of isolated eigenvalues of finite multiplicity, this difference is usually insignificant and often empty (as it is for the main examples below).

In section 3 we describe the source of our principal examples of self adjoint operators. We show how one should 'discretize' the canonical commutation relations so as to preserve the uncertainty principle, and relate the resulting Schrödinger operators to the tridiagonal operators considered in section 4. The one-parameter family of C^*-algebras generated by the discretized canonical commutation relations turns out to be the one-parameter family of noncommutative spheres of Bratteli, Elliott, Evans and Kishimoto [9], [10], [11]. In our case the parameter is related to the numerical step size.

In section 4 we clarify the role of C^*-algebras in numerical problems of this kind. In particular, the C^*-algebra s associated with a broad class of tridiagonal operators are simple C^*-algebra s having a unique tracial state. The tracial state plays an essential role in describing the limit of the eigenvalue distributions of the approximating sequence of finite dimensional truncations of the basic operator.

While there are some new results below, what follows is primarily an exposition of the results of several recent papers [1], [2], [3], [5].

2. Filtrations and degree. Let H be a Hilbert space. A *filtration* of H is an

increasing sequence

$$\mathcal{F} = \{H_1 \subseteq H_2 \subseteq \dots\}$$

of finite dimensional subspaces H_n of H with the property that

$$\lim_{n\to\infty} \dim H_n = \infty.$$

The filtration $\mathcal{F}$ is called *proper* or *improper* according as the union $\cup H_n$ is dense in H or is not dense in H. In general, we will write P_n and P_+ for the projections onto the subspaces H_n and $\overline{\cup H_n}$ respectively.

The simplest filtrations are associated with orthonormal sets in H. For example, if $\{e_n : n = 1, 2, \dots\}$ is an orthonormal set then

$$H_n = [e_1, e_2, \dots, e_n], \qquad n = 1, 2, \dots \tag{2.1}$$

defines a filtration of H which is proper iff $\{e_n\}$ is an orthonormal basis. If, on the other hand, we are given a bilateral orthonormal basis $\{e_n : n = 0, \pm 1, \pm 2, \dots\}$ for H, then

$$H_n = [e_n, e_{-n+1}, \dots, e_n]$$

defines a proper filtration in which the dimensions increase in jumps of 2. Moreover, there is a natural *improper* filtration associated with such a bilateral basis, namely $\mathcal{F}^+ = \{H_1^+ \subseteq H_2^+ \subseteq \dots\}$ where

$$H_n^+ = [e_0, e_1, \dots, e_n], \qquad n = 1, 2, \dots.$$

The spaces H_n^+ span a proper subspace H_+ of H. This example of an improper filtration is associated with 'unilateral' sections. That is to say, the matrix of any operator $A \in \mathcal{B}(H)$ relative to the basis $\{e_n : n \in \mathbb{Z}\}$ is a doubly infinite matrix (a_{ij}), whereas the matrix of the compression

$$P_+ A \restriction_{H_+}$$

is a singly infinite submatrix of (a_{ij}). While these are the main examples of filtrations for our purposes here, filtrations in general are allowed to have very irregular jumps in dimension.

Given any filtration $\mathcal{F} = \{H_n : n \geq 1\}$ of H, we introduce the notion of degree of an operator (relative to $\mathcal{F}$) as follows.

Definition 2.2. *The degree of $A \in \mathcal{B}(H)$ is defined by*

$$\deg(A) = \sup_n \ \mathit{rank}(P_n A - A P_n).$$

The degree of an operator can be any nonnegative integer or $+\infty$, and it is clear that $\deg(A) = \deg(A^*)$. Operators of finite degree are an abstraction of band-limited matrices. For example, suppose we have a proper filtration arising from an orthonormal basis as in 2.1. If the matrix (a_{ij}) of an operator $A \in \mathcal{B}(H)$ relative to this basis satisfies

$$a_{ij} = 0, \quad \text{when } |i - j| > k$$

then $\deg(A) \leq k$. The degree function has a number of natural properties, the most notable being

$$\deg(AB) \leq \deg(A) + \deg(B).$$

The set of all operators of finite degree is a unital $*$-subalgebra of $\mathcal{B}(H)$ which is dense in the strong operator topology [3].

There is a somewhat larger $*$-algebra of operators that one can associate to a filtration $\mathcal{F}$. This is a Banach $*$-algebra relative to a new norm, and it plays a key role in the results to follow. This Banach algebra is defined as follows. Suppose that an operator $A \in \mathcal{B}(H)$ can be decomposed into an infinite sum of finite degree operators

$$A = A_1 + A_2 + \dots \tag{2.3}$$

where the sequence A_n satisfies the condition

$$s = \sum_{n=1}^{\infty} (1 + \deg(A_n)^{1/2}) \|A_n\| < \infty. \tag{2.4}$$

Notice that the sum indicated in 2.3 is absolutely convergent in the operator norm since 2.4 implies

$$\sum_{n=1}^{\infty} \|A_n\| \leq s < \infty.$$

We define $|A|_{\mathcal{F}}$ to be the infimum of all numbers s associated with decompositions of A of this kind. If A cannot be so decomposed then $|A|_{\mathcal{F}}$ is defined as $+\infty$. We define

$$\mathcal{D}_{\mathcal{F}} = \{A \in \mathcal{B}(H) : |A|_{\mathcal{F}} < \infty\}.$$

$(\mathcal{D}_{\mathcal{F}}, |\cdot|_{\mathcal{F}})$ is a unital Banach algebra which contains all finite degree operators, and the operator adjoint defines an isometric involution in $\mathcal{D}_{\mathcal{F}}$. The two norms currently in view are related by

$$\|A\| \leq |A|_{\mathcal{F}}.$$

While it is not so easy to calculate the norm in $\mathcal{D}_{\mathcal{F}}$, it is usually very easy to obtain effective estimates. For example, let $\mathcal{F}$ be a proper filtration associated with a unilateral orthonormal basis as in 2.1, let A be an operator on H and let (a_{ij}) be the matrix of A relative to this basis. Letting

$$d_k = \sup_i \ |a_{i,i+k}|$$

denote the supnorm of the kth diagonal, $k = 0, \pm 1, \pm 2, \dots$, then we have

$$|A|_{\mathcal{F}} \leq \sum_{k=-\infty}^{+\infty} (1 + (2|k|)^{1/2}) d_k.$$

See [3]. Thus, A will belong to $D_{\mathcal{F}}$ whenever the diagonals of (a_{ij}) die out fast enough so that

$$\sum^{+\infty} |k|^{1/2} d_k < \infty.$$

We now indicate the role of the Banach algebra $D_{\mathcal{F}}$ in computing spectra. Let $A \in \mathcal{B}(H)$ be a self adjoint operator and consider the sequence of matrices A_n obtained by compressing A along the filtration $\mathcal{F} = \{H_1 \subseteq H_2 \subseteq \dots\}$:

$$A_n = P_n A \restriction_{H_n} .$$

We are interested in certain asymptotic quantities that can be computed (at least in principle) from the sequence of finite dimensional spectra $\sigma(A_1), \sigma(A_2), \dots$. The simplest one is the set Λ, which consists of all real numbers with the property that there is a sequence of eigenvalues $\lambda_n \in \sigma(A_n)$, $n = 1, 2, \dots$ such that

$$\lim_{n\to\infty} \lambda_n = \lambda.$$

Λ is in some sense the set of *limit points* of the sequence of sets $\sigma(A_1), \sigma(A_2), \dots$. Notice however that Λ is smaller than the topological limit superior of sets because limits along subsequences of $\sigma(A_1), \sigma(A_2), \dots$ do not qualify for membership in Λ. It is easy to see that Λ is closed, and in general Λ contains the spectrum of A [3]. In particular, Λ is never empty. The points of Λ are classified as follows.

For every subset $S \subseteq \mathbb{R}$ and every $n = 1, 2, \dots$ we write $N_n(S)$ for the number of eigenvalues of A_n which belong to S...and of course one counts multiple eigenvalues according to their multiplicity.

Definition 2.5. *A real number λ is called a transient point if there is an open set U containing λ such that*

$$\sup_{n\geq 1} N_n(U) \leq M < \infty.$$

λ is called an essential point if for every open set U containing λ we have

$$\lim_{n\to\infty} N_n(U) = \infty.$$

Remarks. With every transient point λ of Λ there is an associated pair of positive integers $p \leq q$ with the property that for every sufficiently small neighborhood U of λ one has the behavior

$$p \leq N_k(U) \leq q$$

for large enough $k \geq n = n_U$, and moreover both extreme values p and q are taken on infinitely many times by the sequence $N_1(U), N_2(U), \dots$.

The set of all essential points is a subset of Λ which we denote by Λ_e. Again, it can be seen that Λ_e *is a closed set which contains the essential spectrum of* A [3]. At this level of generality, there does not appear to be much more that one can say. For instance, there are examples which show that the both inclusions $\sigma(A) \subseteq \Lambda$ and $\sigma_e(A) \subseteq \Lambda_e$ can be proper (see the appendix of [3]). Other examples show that Λ can contain points which are neither essential nor transient; for every small neighborhood U of such a point one can find subsequences $n_1 < n_2 < \dots$ for which the sequence of positive integers $N_{n_1}(U), N_{n_2}(U), \dots$ stays bounded, and other subsequences $m_1 < m_2 \dots$ such that $N_{m_k}(U) \to \infty$ as $k \to \infty$. Fortunately, the following result implies that in the reasonable cases we will not find this kind of instability.

We can now state our main general result, which shows how one must choose a filtration in order to compute the essential spectrum of a self adjoint operator.

Theorem 2.6. *Let $\mathcal{F}$ be a proper filtration and let A be a self adjoint operator which belongs to the Banach $*$-algebra $\mathcal{D}_{\mathcal{F}}$. Then Λ_e coincides with the essential spectrum of A. Moreover, every point of Λ is either transient or essential.*

Remarks. In the following section we will encounter tridiagonal operators A which are defined in terms of a bilateral orthonormal basis $\{e_n : n = 0, \pm 1, \pm 2, \dots\}$ by

$$Ae_n = e_{n-1} + d_n e_n + e_{n+1}, \tag{2.7}$$

where d_n represents a bounded sequence of reals. Theorem 2.6 shows how the essential spectrum of A can be computed in terms of the eigenvalue distributions of the sequence of $(2n+1) \times (2n+1)$ matrices obtained by compressing A along the sequence of subspaces $H_n = [e_{-n}, e_{-n+1}, \dots, e_{n-1}, e_n]$, $n = 1, 2, \dots$. While Theorem 2.6 says nothing about *rates* of convergence, our experience with the operators of section 4 has shown that convergence is rapid; in fact, it is fast enough to allow the construction of excellent pictures of $\sigma_e(A)$ on desktop computers in a minute or two [4]. Nevertheless, there remains an important problem of obtaining an appropriate definition of the "rate" of convergence of such approximations, and the estimation of this rate. The paper [3] does not address these issues of error definition and estimation.

In carrying out computations, it is usually more convenient to deal not with the above "bilateral" sections A_n but with smaller "unilateral" sections. More precisely, these are defined in terms of an *improper* filtration $\{H_1^+ \subseteq H_2^+ \subseteq \dots\}$, $H_n^+ = [e_1, e_2, \dots, e_n]$, and the corresponding compressions of the operator A

$$A_n^+ = P_n^+ A \restriction_{H_n^+},$$

P_n^+ denoting the projection onto H_n^+. Since the filtration $\{H_n^+\}$ is improper, Theorem 2.6 does not allow one to draw conclusions about the essential spectrum of A, but rather the essential spectrum of the operator A^+ obtained by compressing A to the subspace H^+ generated by $\cup_n H_n^+$. Thus there remains a significant problem of relating the essential spectrum of A to that of A^+. These issues will be taken up in section 4 below.

3. Discretized Schrödinger operators. In this section we will indicate how a one-dimensional quantum system should be discretized in order to carry out numerical computations. We will find that the "discretized" canonical commutation relations generate a C^*-algebra which is isomorphic to one of the noncommutative spheres of Bratteli, Elliott, Evans and Kishimoto (with parameter related to the numerical step size), and we will find that the resulting discretized Hamiltonian is a bounded self-adjoint operator which is amenable to the methods of the preceding section.

Most one-dimensional quantum systems are modelled on the Hilbert space $L^2(\mathbb{R})$. The canonical operators are the unbounded self-adjoint operators P, Q defined on appropriate domains in $L^2(\mathbb{R})$ by

$$P = \frac{1}{i}\frac{d}{dx}, \tag{3.1}$$

Q = Multiplication by x

They obey the canonical commutation relations on an appropriate common domain

$$PQ - QP = \frac{1}{i}\mathbf{1}.$$

The time development of the system is described by a one-parameter unitary group of the form

$$W_t = e^{itH}, \qquad t \in \mathbb{R},$$

where H is the Hamiltonian of the system

$$H = \frac{1}{2}P^2 + \phi(Q), \tag{3.2}$$

ϕ being a real-valued continuous function of a real variable which represents the potential of the classical system being quantized.

In order to carry out numerical computations one first has to replace the differential operator H with an appropriately discretized version of itself. Moreover, one has to decide how this should be done so as to conform with the basic principles of numerical analysis while at the same time preserving the essential features of quantum mechanics (i.e., the uncertainty principle). In [1] we presented arguments which we believe justify the following procedure.

One first settles on a numerical step size σ. This can be regarded as a small positive rational number, whose size represents the smallest time increment to be used in the difference equations that replace differential equations. One then discretizes *both* operators P and Q, and finally uses the formula 3.2 to define the corresponding discretized version of the Hamiltonian.

In more detail, we replace the differential operator P with the bounded self-adjoint difference operator P_σ defined by

$$P_\sigma f(x) = \frac{f(x+\sigma) - f(x-\sigma)}{2i\sigma}, \qquad x \in \mathbb{R}.$$

Noting that the one-parameter group of translations $V_t f(x) = f(x+t)$ is generated by P in the sense that $V_t = e^{itP}, t \in \mathbb{R}$, we have

$$P_\sigma = \frac{1}{2i\sigma}(e^{i\sigma P} - e^{-i\sigma P}) = \frac{1}{\sigma}\sin(\sigma P).$$

Now we must discretize Q but we must be careful to do it in a way that preserves the uncertainty principle insofar as that is possible. In section 3 of [1], we argued that this requirement imposes a very strong restriction on the possible choices for the discretized Q, and that in fact the only "correct" choice is given by

$$Q_\sigma = \frac{1}{2i\sigma}(e^{i\sigma Q} - e^{-i\sigma Q}) = \frac{1}{\sigma}\sin(\sigma Q).$$

More explicitly, we have

$$Q_\sigma f(x) = \frac{1}{\sigma}\sin(\sigma x) f(x), \qquad x \in \mathbb{R},\ f \in L^2(\mathbb{R}).$$

The resulting discretized Hamiltonian is then defined as follows:

$$H_\sigma = \frac{1}{2}P_\sigma^2 + V(Q_\sigma). \tag{3.3}$$

Once we have the operator H_σ we are in position to carry out numerical computations with the quantum system. For example, if the system is described at time t by a wave function $f \in L^2(\mathbb{R})$ then the state of the system at time $t + \Delta t$ is approximated by the wave function

$$g = (\mathbf{1} + i\Delta t H_\sigma)f = f + i\Delta t H_\sigma f.$$

We caution the reader that, while the preceding formula is convenient for illustrating one way to make use of the discretized Hamiltonian, it must be modified appropriately in order to correctly model the dymanical group in practice because the operator $f \mapsto g$ is not unitary. Readers interested in carrying out numerical computations can find a discussion of closely related issues in [14, pp 662–663].

Let $\mathcal{D}_\sigma$ be the C^*-algebra generated by the set of operators $\{P_\sigma, Q_\sigma\}$. $\mathcal{D}_\sigma$ is the norm-closed linear span of all finite products of terms involving either P_σ or Q_σ. It is not obvious that $\mathcal{D}_\sigma$ contains the identity operator but that is the case. $\mathcal{D}_\sigma$ is the discretized counterpart of the algebra of observables, and notice that it contains the operator H_σ. Thus it is important to understand the structure of $\mathcal{D}_\sigma$.

In fact, $\mathcal{D}_\sigma$ is a simple unital C^*-algebra which is isomorphic to one of the non-commutative spheres of Bratteli et al [9, 10, 11]. Moreover, while the operators P_σ, Q_σ no longer satisfy the canonical commutation relations, they do obey a more subtle discretized form of the CCRs, and more generally it is the universal C^*-algebra associated with these "discretized" CCRs that is naturally associated with the non-commutative spheres. The reader is referred to [2] for a detailed discussion of these and related issues.

In particular, if one is interested in computing the spectrum of H_σ then one is free to choose any convenient representation of $\mathcal{D}_\sigma$ and compute the spectrum of H_σ in that representation. Since $\mathcal{D}_\sigma$ is simple, the spectrum does not depend on the representation chosen. Actually, the most convenient realization of H_σ is one in which it is a tridiagonal operator. In this case, it is more appropriate to work with a subalgebra of $\mathcal{D}_\sigma$ which contains H_σ. The precise statement follows.

Proposition 3.4. *Let $\mathcal{A}$ be the C^*-algebra generated by P_σ^2 and Q_σ, and let K be a Hilbert space spanned by a bilateral orthonormal set $\{e_n : n \in \mathbb{Z}\}$. Then there is a faithful representation $\pi : \mathcal{A} \to \mathcal{B}(K)$ such that $\pi(H_\sigma)$ has the form*

$$\pi(H_\sigma) = aT + b\mathbf{1} \tag{3.5}$$

where $a = 1/8\sigma^2$, $b = -1/4\sigma^2$, and T is the tridiagonal operator

$$Te_n = e_{n-1} + 8\sigma^2\phi(\frac{1}{\sigma}\sin(2n\sigma))e_n + e_{n+1}, \tag{3.6}$$

$n = 0, \pm 1, \pm 2, \dots$.

proof. Consider the unitary operators U, V defined by

$$Uf(x) = e^{i\sigma x}f(x)$$
$$Vf(x) = f(x + \sigma)$$

Then

$$P_\sigma = \frac{1}{2i\sigma}(V - V^{-1}),$$
$$Q_\sigma = \frac{1}{2i\sigma}(U - U^{-1}),$$

and notice that

$$P_\sigma^2 = -\frac{1}{4\sigma^2}(V^2 + V^{-2}) + \frac{1}{2\sigma^2}.$$

Let $\mathcal{B}$ be the C^*-algebra generated by U and V^2. Clearly $\mathcal{A}$ is contained in $\mathcal{B}$, and because of the commutation relation

$$V^2U = e^{2i\sigma^2}UV^2$$

and the fact that σ is a positive rational number, it follows that $\mathcal{B}$ is an irrational rotation C^*-algebra. We will define a representation π_1 of $\mathcal{B}$ on K; the required representation of $\mathcal{A}$ is obtained by restriction.

In order to specify a representation of $\mathcal{B}$ on K, it is sufficient to specify a pair of unitary operators S, D on K satisfying

$$SD = e^{2i\sigma^2}DS. \tag{3.7}$$

π_1 is then uniquely defined by specifying that $\pi_1(V^2) = S$, $\pi_1(U) = D$. Let

$$Se_n = -e_{n-1},$$
$$De_n = e^{2in\sigma^2}e_n$$

$n = 0, \pm 1, \pm 2, \ldots$. Clearly S and D are unitary operators and the reader can verify 3.7 directly. Hence there is a representation π_1 of $\mathcal{B}$ with the stated properties. Noting that

$$\pi_1(P_\sigma^2) = \pi_1(-\frac{1}{4\sigma^2}(V^2 + V^{-2}) + \frac{1}{2\sigma^2}\mathbf{1})$$
$$= -\frac{1}{4\sigma^2}S - \frac{1}{4\sigma^2}S^{-1} + \frac{1}{2\sigma^2}\mathbf{1}$$

and that $\pi_1(Q_\sigma)$ is the diagonal operator

$$\pi_1(Q_\sigma)e_n = \frac{1}{2i\sigma}(e^{2in\sigma^2} - e^{-2in\sigma^2})e_n = \frac{1}{\sigma}\sin(2n\sigma^2)e_n,$$

we may conclude that

$$\pi_1(\phi(Q_\sigma))e_n = \phi(\frac{1}{\sigma}\sin(2n\sigma^2))e_n$$

for every $n = 0, \pm 1, \pm 2, \ldots$. Combining these two formulas, we find that the image of H_σ is given by

$$\pi_1(H_\sigma) = \frac{1}{2}\pi_1(P_\sigma^2) + \pi_1(\phi(Q_\sigma)).$$

which has the form spelled out in 3.5 and 3.6 □

Remark 3.8. Consider the diagonal sequence

$$d_n = 8\sigma^2\phi(\frac{1}{\sigma}\sin(2n\sigma^2)), \qquad n \in \mathbb{Z}$$

appearing in the formula 3.6. We want to point out that if the function ϕ is continuous and not constant on the interval $[-\frac{1}{\sigma}, +\frac{1}{\sigma}]$ and if σ^2 is not a rational multiple of π, then the sequence (d_n) is *almost periodic* but *not periodic*. Indeed, the sequence $n \mapsto \sin(2n\sigma^2)$ is almost periodic because it is a linear combination of complex exponentials of the form $e^{i\alpha n}$ where α is a real number. Since the set of all almost periodic sequences form a commutative C^*-algebra it is closed under the continuous functional calculus, and therefore the sequence (d_n) must be almost periodic. Note too that (d_n) cannot be periodic. For if there did exist integers $p \geq 1$ and n such that

$$d_{n+kp} = d_n, \qquad k = 0, \pm 1, \pm 2, \dots$$

then since σ^2 is not a rational multiple of π the numbers

$$\sin(2n\sigma^2 + 2kp\sigma^2), \qquad k \in \mathbb{Z}$$

would fill out a dense set in the interval $[-1, +1]$, and hence ϕ would have to be constant on the interval $[-\frac{1}{\sigma}, +\frac{1}{\sigma}]$.

The material presented in this section leads toward a significant conclusion. *The problem of computing the spectrum of the discretized Hamiltonian of a one dimensional quantum system can be reduced to the problem of computing the spectrum of a self-adjoint tridiagonal operator of the form*

$$Te_n = e_{n-1} + d_n e_n + e_{n+1}, \qquad n \in \mathbb{Z} \tag{3.9}$$

where $\{d_n : n \in \mathbb{Z}\}$ *is a bounded almost periodic sequence of reals which is not periodic.* For such operators one can work with either unilateral sections or bilateral sections, as we will see in the following section. For example, if for $n \geq 1$ we let T_n be the compression of T onto the linear span of $\{e_1, e_2, \dots, e_n\}$ then even though we are in effect working with an improper filtration, one may apply a suitable variation of Theorem 2.6 to conclude that the spectrum of T is the set of all essential points associated with the sequence of self-adjoint matrices $T_1, T_2, \dots$.

In the following section, we will obtain more precise information about the distribution of the eigenvalues of the sequence T_n, $n = 1, 2, \dots$.

4. Limits, simple C^*-algebras, and traces. Let $(d_n)_{n\in\mathbb{Z}}$ be a bounded almost periodic sequence of reals which is *not* periodic and let T be the tridiagonal operator of 3.9

$$Te_n = e_{n-1} + d_n e_n + e_{n+1}, \qquad n \in \mathbb{Z}, \tag{4.1}$$

$\{e_n : n \in \mathbb{Z}\}$ being an orthonormal basis for a Hilbert space H. We will show that the eigenvalue distributions of the $n \times n$ sections of T actually converge (in the weak*-topology of measures on the real line) to a probability measure μ. Thus it

becomes important to understand the nature of this limiting measure μ_T. We show that μ_T is associated with a tracial state on a certain C^*-algebra $\mathcal{A}_T$ associated with T. $\mathcal{A}_T$ certainly contains T but it is much larger than the C^*-algebra generated by T; indeed, $\mathcal{A}_T$ is a simple C^*-algebra having a *unique* tracial state.

Let S be the bilateral shift defined on H by

$$Se_n = e_{n+1} \qquad n \in \mathbb{Z}$$

and let D be the diagonal operator associated with the sequence (d_n),

$$De_n = d_n e_n, \qquad n \in \mathbb{Z}.$$

$\mathcal{A}_T$ is defined as the C^*-algebra generated by both operators D and S. $\mathcal{A}_T$ is a separable unital C^*-algebra which contains T, and of course $\mathcal{A}_T$ depends on the particular choice of diagonal sequence (d_n). When T is a discretized Hamiltonian as in the previous section, $\mathcal{A}_T$ will depend on both the numerical step size σ and the potential ϕ. Nevertheless, in all cases we have

Theorem 4.2. *$\mathcal{A}_T$ is a simple unital C^*-algebra-subalgebra of $\mathcal{B}(H)$ which has a unique tracial state.*

Remark. A *tracial state* of $\mathcal{A}_T$ is a linear functional $\tau : \mathcal{A}_T \to \mathbb{C}$ satisfying

$$\tau(X^*X) \geq 0, \quad and$$
$$\tau(XY) = \tau(YX)$$

for every $X, Y \in \mathcal{A}_T$, and which is normalized so that $\tau(\mathbf{1}) = 1$. Theorem 4.2 is proved in proposition 3.2 of [5].

More generally, suppose we are given an arbitrary concrete C^*-algebra $\mathcal{A} \subseteq \mathcal{B}(H)$. We need to single out the filtrations that are "compatible" with $\mathcal{A}$. Let $\mathcal{F} = \{H_1 \subseteq H_2 \subseteq \dots\}$ be a filtration of H which may be improper, and put

$$H_+ = \overline{\cup_n H_n}.$$

As in section 2 we may speak of the degree of an operator $X \in \mathcal{B}(H)$ relative to the filtration $\mathcal{F}$. Following [3], we say that $\mathcal{F}$ is an $\mathcal{A}$-filtration if the set of finite degree operators which belong to $\mathcal{A}$ is norm-dense in $\mathcal{A}$.

In connection with the operators T of 4.1, we will consider the filtration $\mathcal{F}_T = \{H_n\}$ where $H_n = [e_1, e_2, \dots, e_n]$. This is an improper filtration for which

$$H_+ = [e_1, e_2, \dots].$$

More significantly, we have

Proposition 4.3. *$\mathcal{F}_T$ is an $\mathcal{A}_T$-filtration.*

4.3 is a simple consequence of the fact that the finite degree operators in $\mathcal{A}_T$ form a of $\mathcal{A}_T$, and that the operators D and S have respective degrees 0 and 1 (see the proof of Theorem 3.4 of [5]). For every $n \geq 1$ let T_n be the compression of T to H_n. Relative to the obvious basis for H_n, the matrix of T_n is

$$\begin{pmatrix} d_1 & 1 & 0 & \dots & 0 & 0 \\ 1 & d_2 & 1 & \dots & 0 & 0 \\ 0 & 1 & d_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & d_{n-1} & 1 \\ 0 & 0 & 0 & \dots & 1 & d_n \end{pmatrix}.$$

There are two issues that need to be understood. The first has to do with the relation between operators in $\mathcal{A}_T$ and their compressions to H_+; the second requires relating the trace on $\mathcal{A}_T$ to the limit of the eigenvalue distributions of the sequence of matrices $T_1, T_2, \dots$.

In order to discuss the first of these, we consider a more general setting in which we are given a unital C^*-algebra $\mathcal{A} \subseteq \mathcal{B}(H)$ and an improper filtration $\{H_1 \subseteq H_2 \subseteq \dots\}$. We will consider the space $\mathcal{A}_+$ of all operators on H_+ having the form

$$P_+ A \restriction_{H_+} + K,$$

where $A \in \mathcal{A}$ and K is a compact operator on H_+, P_+ denoting the projection on H_+. We will write $\mathcal{K}_+$ for the algebra of all compact operators on H_+.

Theorem 4.4. *Assume that $\mathcal{A}$ has a unique tracial state τ, let $\{H_1 \subseteq H_2 \subseteq \dots\}$ be an $\mathcal{A}$-filtration and assume that H_+ has the following property*

$$A \restriction_{H_+} = \textit{compact} \implies A = \textit{compact} \tag{4.5}$$

for every operator $A \in \mathcal{A}$. Then $\mathcal{A}_+$ is a C^*-algebra containing $\mathcal{K}_+$ which has a unique tracial state τ_+. τ_+ is related to τ by way of

$$\tau_+(P_+ A \restriction_{H_+} + K) = \tau(A), \qquad A \in \mathcal{A}, K \in \mathcal{K}_+.$$

Moreover, the natural map of $\mathcal{A}$ to the quotient $\mathcal{A}_+/\mathcal{K}_+$ given by

$$A \mapsto P_+ A \restriction_{H_+} + \mathcal{K}_+$$

is an isomorphism of C^*-algebras:

$$\mathcal{A} \cong \mathcal{A}_+/\mathcal{K}_+.$$

Remarks. The argument required here can be found in the proof of Theorem 2.3 of [5]. These results depend on the following relationship that exists between the operators in $\mathcal{A}$ and the projection P_+ associated with an $\mathcal{A}$-filtration:

$$A \in \mathcal{A} \implies P_+ A - A P_+ \in \mathcal{K}$$

see [5, proposition 2.1].

Theorem 4.4 implies that we have a short exact sequence of C^*-algebras

$$0 \to \mathcal{K}_+ \to \mathcal{A}_+ \to \mathcal{A} \to 0.$$

This shows that the structure of $\mathcal{A}_+$ is somewhat analogous to the structure of the Toeplitz C^*-algebra $\mathcal{T}$,

$$0 \to \mathcal{K} \to \mathcal{T} \to C(\mathbb{T}) \to 0,$$

except that in our applications the quotient C^*-algebras $\mathcal{A}_T$ are highly noncommutative.

Finally, we remark that the hypothesis 4.5 is satisfied for our examples $\mathcal{A}_T$ because $\mathcal{A}_T$ is a simple C^*-algebra with unit and H_+ is infinite dimensional (see the proof of Theorem 2.4 of [5]).

Now we can define the measure μ_T alluded to at the beginning of this section. Let τ be the unique tracial state of $\mathcal{A}_T$. Using the functional calculus for bounded self-adjoint operators, we can define a positive linear functional on $C_0(\mathbb{R})$ by

$$f \in C_0(\mathbb{R}) \mapsto \tau(f(T)).$$

By the Riesz-Markov theorem, there is a unique positive measure μ_T on $\mathbb{R}$ such that

$$\int_{-\infty}^{+\infty} f(x)\, d\mu_T(x) = \tau(f(T)), \qquad f \in C_0(\mathbb{R}).$$

μ_T is obviously a probability measure whose support is contained in the spectrum of T. μ_T is called the *spectral distribution* of T. Because $\mathcal{A}_T$ is simple τ must be a faithful trace, and hence the closed support of μ_T is *exactly* the spectrum of T.

The preceding discussion, together with the general results of [3, section 4] can be applied to obtain the following result, which is Theorem 3.4 of [5].

Theorem 4.6. *For every positive integer n let $\lambda_1^n < \lambda_2^n < \cdots < \lambda_n^n$ be the eigenvalue list of the symmetric $n \times n$ matrix*

$$\begin{pmatrix} d_1 & 1 & 0 & \dots & 0 & 0 \\ 1 & d_2 & 1 & \dots & 0 & 0 \\ 0 & 1 & d_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & d_{n-1} & 1 \\ 0 & 0 & 0 & \dots & 1 & d_n \end{pmatrix}. \tag{4.7}$$

Then for every $f \in C_0(\mathbb{R})$ we have

$$\lim_{n\to\infty} \frac{1}{n}(f(\lambda_1^n) + f(\lambda_2^n) + \dots, + f(\lambda_n^n)) = \int_{-\infty}^{+\infty} f(x)\, d\mu_T(x).$$

Remarks. Theorems 4.6 and 2.6 together provide rather precise information about the rate at which the eigenvalues of the matrices 4.7 accumulate at points in and out of the spectrum of T. For example, let $\lambda \in \sigma(T)$ and let I be an open interval containing λ. Then $\mu_T(I) > 0$, and if α and β are chosen close to $\mu_T(I)$ in such a way that $\alpha < \mu_T(I) < \beta$, then the number $N_n(I)$ of eigenvalues of T_n which belong to I will satisfy the inequalities

$$\alpha n \le N_n(I) \le \beta n$$

for all sufficiently large n.

For the operators T of 4.1, it is not hard to show that the essential spectrum of T is identical with $\sigma(T)$. Thus we can apply Theorem 2.6 above to conclude that if λ does *not* belong to $\sigma(T)$ then for every sufficiently small open interval containing λ, the sequence of numbers $N_1(I), N_2(I), \dots$ actually remains bounded. This behavior is quite visible in the pictures generated by the program [4].

Some additional remarks relating to computational issues can be found in the concluding paragraphs of [5].

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